Post-Processing Data

The Lou data analysis nodes (LDANs) provide dedicated PBS resources to perform post-processing tasks on your Lou mass storage data. You can also use them for performing pre-processing or post-processing tasks on active Pleiades, Aitken, or Electra data. The LDANs can be accessed only through PBS jobs in which resources are dedicated to the job owner.

The LDANs contain Intel Xeon Gold 6154 "Skylake" processors, equipped with more memory than the Electra Skylake nodes, as follows:

- Each Idan[11-12] has 36 cores and 768 GB of memory
- Each Idan[13-14] has 36 cores and 1.5 TB of memory

The Lou, Lustre, and Pleiades home filesystems are mounted on the LDANs. You can access them in a PBS job running on an LDAN by using the following paths:

Lou

/u/username

Lustre:

/nobackup/username

Pleiades:

/pleiades/u/username

#### **Software Modules**

All of the software packages that you use on the Pleiades front-end (PFE) nodes or Pleiades/Aitken/Electra compute nodes are also available on the LDANs. However, both the Lou front-end (LFE) nodes and LDANs use startup files from your Lou home directory rather than your Pleiades home directory.

Therefore, if your PBS jobs rely on loading specific software modules or environment variables in your Pleiades system startup files (such as .cshrc), in order to run them on the LDANs you must modify your startup files on Lou to load the <u>modules</u> and set appropriate <u>environment variables</u>.

#### **Running PBS Jobs on LDANs**

The PBS server for the LDANs is pbspl1. To use the LDANs, submit your jobs to the ldan queue. Each job can use only *one* LDAN for up to *three days*, and each user can have a maximum of *two jobs* running simultaneously.

Before You Begin: If you want to process archive data that has been migrated offline to tape, use the <u>Data Migration Facility</u> command dmget to migrate the data back to disk before submitting jobs to the LDANs.

## **Submitting Your PBS Job**

You can submit interactive PBS jobs to the LDANs from either the LFEs or the PFEs. You can submit PBS job scripts from either your Lustre home filesystem (/nobackup/username) or your Lou home filesystem (/u/username).

WARNING: Do not submit job scripts from the Pleiades home filesystem, because PBS error and output files cannot be copied back there from the LDANs.

Use the :mem=xxxGB attribute to specify how much memory you need for your job. This will instruct PBS to allocate an appropriate LDAN.

Note: Keep in mind that the amount of memory on a node that is available for your job is slightly less than the total physical memory, because the system kernel can use up to 4 GB of memory in each node.

## Sample PBS Script

#PBS -lselect=1:ncpus=36:mem=750GB #PBS -lwalltime=2:00:00 #PBS -q Idan

### Remember to load necessary modules ### or set environment variables that you need

module load xxx

### Note that the default directory a PBS job ### is in when it starts is the Lou home filesystem. ### Change directory to the appropriate directory ### for your pre- or post- processing work.

cd \$PBS\_O\_WORKDIR

### If your executable for pre- or post- processing ### is located under your Pleiades home filesystem, ### use the pathname /pleiades/u/username/bin/....

### do not use the pathname /u/username/bin/...

/pleiades/u/username/bin/your\_processing\_code < input > output

## **Running Graphics Applications on LDANs**

If you want to run graphics applications that consume enough memory to require one of the larger-memory LDANs, submit an interactive PBS job from one of the LFEs that specifies mem=1040GB. For example:

Ife% qsub -I -q Idan -Iselect=1:mem=1040GB,walltime=1:00:00

This will provide you with an LDAN for the duration of the specified wall time. Then, from any other terminal window, you can use SSH to connect directly to the LDAN assigned to your job, and run your graphics application interactively. If you have SSH passthrough set up, you can even SSH directly in to the LDAN from your workstation by adding the LDANs as allowed SSH passthrough targets in your .ssh/config file.

To run graphics applications directly from a PBS session submitted from an LFE, you need to export your DISPLAY environment by adding the -X option to the qsub command, as follows:

Ife% qsub -I -X -q Idan -Iselect=1:mem=750GB,walltime=1:00:00

If you are a remote user, you can also explore using Virtual Network Computing (VNC) to connect to NAS systems.

The PFEs are the front-end systems for Pleiades, Aitken, Electra, and Endeavour. They provide an environment that enables quick turnaround for tasks such as file editing, file transferring, compiling, and short debugging/testing sessions, as well as for batch job submissions via PBS to a subset of the Pleiades compute nodes, or to Aitken, Electra, to Endeavour.

WARNING: The PFEs use Intel Sandy Bridge processors. If you use a PGI compiler to build your executable on the PFEs, be aware that by default the executable is optimized for the Sandy Bridge microarchitecture (which includes Sandy Bridge and Ivy Bridge) and will not necessarily execute on the compute node processors. See <u>PGI Compilers and Tools</u> for information on generating a single executable that will work on all processor types.

You cannot use SSH to access the compute nodes except for the subset of nodes your PBS job is running on.

## **Pre-Processing and Post-Processing Data**

For pre- and post-processing applications such as <u>Tecplot</u>, <u>IDL</u>, and <u>MATLAB</u>, we recommend using the <u>Lou data analysis nodes</u> (LDANs). You can request the LDANs in the qsub command line. The Lou home filesystems, Pleiades home filesystems, and /nobackup filesystems are all mounted on the LDANs.

#### **Restrictions on Front-End Systems**

MPI (Message Passing Interface) jobs are *not* permitted to run on the PFEs. In addition, you will be notified by email if a job running on a PFE exceeds 27 GB.

Before starting a large-memory session, it is a good idea to make sure there is enough memory available. You can run thetop command, hit "M", and check under the "RES" column for other large memory applications that may be running.

#### File Transfers to Mass Storage

The /nobackup filesystems are mounted on Lou, so the easiest way to transfer files between Pleiades and Lou is to initiate a command such as shiftc, cp, mcp, or tar on Lou. For example:

lou% shiftc /nobackup/username/filename \$HOME

If you initiate the transfer from Pleiades, you can use the commands scp or shifts to transfer files between a PFE and Lou. For very large file transfers, we recommend the NAS-developed <a href="Shift tool">Shift tool</a> (shifts).

 $\label{file:prop:compute} \ \ \text{File transfers from the compute nodes to Lou must first go through one of the PFEs. }$ 

When sending data to Lou, keep your largest individual file size under 1 terabyte (TB). Files larger than 1 TB will occupy all of the tape drives, preventing other file restores and backups.

# **Licensed Application Software**

## **Licensed Application Software: Overview**

There are a few licensed applications available for your use on NAS systems. You can find these in the/nasa directory.

The available licenses were either purchased by NAS—with the justification that many users need the particular applications—or by users themselves. If you would like to use a licensed application that is not yet available on NAS systems, you may need to purchase the license yourself.

#### Interactive Data Language (IDL)

Interactive Data Language (IDL) is a programming language for data analysis, visualization, and cross-platform application development. IDL combines tools for many types of projects, from "quick-look," interactive analysis and display to large-scale commercial programming projects.

NAS currently has IDL development licenses that allow 10 users to use the tool at the same time. Each license allows a single user to run multiple IDL sessions with the same session display simultaneously. Follow these steps to take advantage of this feature:

- 1. Use SSH to connect to a PFE.
- 2. Check the DISPLAY variable of the PFE, and launch multiplexterm sessions to run in the background. For example:

```
pfe25% echo $DISPLAY
pfe25:83.0
pfe25% xterm&
pfe25% xterm&
pfe25% xterm&
```

3. In each xterm window, check the DISPLAY variable to confirm that it has the same number that was shown in the original window. Load an IDL module, then launch the idl command. For example:

```
pfe25% echo $DISPLAY
pfe25:83.0
pfe25% module load idl/8.1
pfe25% idl
IDL>
```

In the example above, a single user occupies only one IDL license rather than three licenses by ensuring that the IDL sessions are running in three separate xterm windows that all have the same DISPLAY number.

Use one of the following methods to view how many licenses are currently in use:

- Run /u/scicon/tools/bin/check\_licenses -i
- Load an IDL module and run the lmstat -a command

WARNING: You must quit IDL and release the license when you are done. Keeping the license in use when you are not actively using IDL prevents others who need access to IDL from doing useful work.

If you cannot use IDL because all licenses are currently being used, try again at a later time. If you notice that multiple licenses are occupied by the same user, please contact the NAS Control Room at (800) 331-8737, (650) 604-4444, or by email at <a href="mailto:support@nas.nasa.gov">support@nas.nasa.gov</a>.

For more information, see:

- NAS IDL License Policy
- IDL Documentation
- IDL Programming Language (Wikipedia)

#### **MATLAB**

MATLAB is a numerical computing environment and programming language, created by MathWorks, that enables you to easily manipulate matrices, plot functions and data, implement algorithms, create user interfaces, and interface with programs in other languages. Although MATLAB specializes in numerical computing, an optional toolbox interfaces with the Maple symbolic engine, allowing it to be part of a full computer algebra system.

A total of 16 licenses are available to use on either NAS HPC systems or NAS-supported desktop systems. To find out how many licenses are currently in use, run:

/u/scicon/tools/bin/check\_licenses -m (view general licenses only)

/u/scicon/tools/bin/check\_licenses -M (view general licenses and compiler/toolboxes)

Then, load a MATLAB module:

% module load matlab/2016b

See the following websites for more information about MATLAB software:

- MATLAB documentation (MathWorks)
- MATLAB (Wikipedia)

See the following Knowledge Base articles for more information about NAS MATLAB licenses:

- MATLAB License Policy
- Using NAS MATLAB Licenses

#### **Tecplot**

Two Tecplot products are available on NAS systems: Tecplot 360 and Tecplot Chorus.

## **Tecplot 360**

Tecplot 360 is a computational fluid dynamics and numerical simulation visualization software program used for post-processing simulation results. Common tasks associated with post-processing analysis of flow solvers (for example, Fluent, STAR-CD, OpenFOAM) include:

- Calculating grid quantities (such as aspect ratios, skewness, orthogonality, and stretch factors)
- Normalizing data; deriving flow field functions (such as pressure coefficient or vorticity magnitude)
- Verifying solution convergence
- Estimating the order of accuracy of solutions
- Interactively exploring data through cut planes (slices through a region), iso-surfaces (3D maps of concentrations), particle paths (dropping an object in the "fluid" and watching where it goes)

The NAS Tecplot 360 license does not restrict the number of instances of Tecplot 360 that can be run concurrently.

TIP: If you are having problems running Tecplot through VNC, you can try running it with the -mesa option, which uses software rendering.

## **Tecplot Chorus**

Tecplot Chorus is a simulation analytics framework that unites physics visualization with data management and analytics in a single environment.

Currently, one Tecplot Chorus license is available to use on Pleiades or NAS-supported desktop systems.

For more information, see:

- Tecplot product documentation
- Tecplot (Wikipedia)

## **Modules and Packages**

#### Software on NAS Systems

Software programs on NAS systems are managed as modules or packages. Available programs are listed in tables below.

Note: The name of a software module or package may contain additional information, such as the vendor name, version number, or what compiler/library is used to build the software. For example:

- comp-intel/2020.4.304 Intel Compiler version 2020.4.304
- mpi-hpe/mpt.2.25 HPE MPI library version 2.25
- netcdf/4.4.1.1\_mpt NetCDF version 4.4.1.1, built with HPE MPT

#### **Modules**

Use the module avail command to see all available software modules. Run module whatis to view a short description of every module. For more information about a specific module, run module help *modulename*.

See <u>Using Software Modules</u> for more information.

Available Modules (as of December 20, 2021)

ModuleFunctionboostC++ library

cdo Climate and NWP data analysis tool comp-aocc AMD Optimizing C/C++ Compiler

comp-intel Intel Compiler

cuda NVIDIA parallel computing platform and programming model

dakota Software toolkit from Sandia fieldview Data visualization & analysis tool

firefox Web browser
gcc C/C++ compiler
hdf4 I/O library & tools
hdf5 I/O library & tools

idl Data visualization & analysis tool

mathematica System & language for mathematical application

matlab Numerical computing environment & programming language

metis Graph, mesh, & hypergraph partitioning software

mpi-hpe HPE MPI library mpi-intel Intel MPI library

ncl NCAR Command Language

nco NetCDF Operators

ncview Visual browser for NetCDF files

netcdf I/O library

nvhpc NVIDIA HPC Software Development Kit octave Numerical computations language

openfoam Open source CFD software

pagecache-management Tool for limiting page cache usage

paraview Data analysis and scientific visualization application

parmetis Math/numerical library

petsc Portable, Extensible Toolkit for Scientific Computation
pkgsrc NetBSD Package Source collection of software packages

python3 Programming language (version 3) scicon Tools created by NAS Scicon team

NAS in-house utility for synchronization and visualization of arbitrary

streams

singularity HPC container platform szip Compression library

tecplot Data visualization & analysis tool

totalview Debugger

vtune Performance analysis tool

x2go Open source remote desktop software for Linux xxdiff Graphical file & directories comparison & merge tool

## Packages in the NetBSD Package Source Collection (pkgsrc)

Many software programs are now managed as packages on NAS systems, via the NetBSD Package Source Collection. To use a package, you must first access the current package collection by loading the pkgsrc module, which is listed in the Modules table.

See <u>Using Software in the NetBSD Packages Collection</u> for more information.

#### Partial list of NetBSD Packages in pgksrc/2021Q2

Module Function

bioperl Perl tools for computational molecular biology

bison GNU yacc(1) replacement blas Basic Linear Algebra System

bmake Portable (autoconf) bersion of NetBSD "make" utility bzr Bazaar open source distributed version control system

clang C language family front-end for LLVM cscope Interactive C program browser

fetch Client to fetch URLs

ffmpeg4 Decoding, encoding, & streaming software (v4.x)

fftw Fast C routines to compute DFTs

gdal Translator library for raster geospacial data formats gettext Tools for providing messages in different languages

git GIT version control suite meta-package

GMT Generic Mapping Tools

gnuplot Portable, interactive function-plotting utility

grace GRaphing, Advanced Computation & Exploration of data GraphicsMagick X application for displaying & manipulating images

h5utils Utilities for conversion to/from HDF5
hdf5-c++ New generation HDF C++ wrappers
htop Enhanced version of "top" utility

ImageMagick Package for display & interactive image manipulation

Irzip Long range ZIP or Lzma RZIP

lz4 Extremely fast compression algorithm

Izop Fast file compressor similar to gzip, using the LZO library mercurial Fast, lightweight source control management system

metis Unstructured graph partitioning & sparse matrix ordering system

mg Small, fast, public domain Emacs-style editor

mono Open-source implementation of .NET Development Framework

nano Small, friendly text editor (a replacement for Pico)

ncview Visual browser for netCDF format files

netcdf-fortran Fortran support for NetCDF

nvi Berkeley nvi with additional features

pbzip2 Parallel implementation of bzip2 block-sorting file compressor

pkgfind Find packages by package name in pkgsrc qgis Geographic information system (GIS)

R Statistical language for data analysis & graphics

rhash Calculate/check CRC32, MD5, SHA1, GOST, or other hash sums

ruby Ruby programming language tkcvs TcI/Tk front-ends to CVS & diff

tmux BSD-licensed terminal multiplexer (GNU screen alternative)

valgrind Debugging & profiling tools

vtk Visualization toolkit

wget Retrieve files from the internet via HTTP & FTP

#### **Using Software Packages in pkgsrc**

The NetBSD Packages Collection (pkgsrc) is a third-party software package management system for Unix-like operating systems. Among the over 17,000 packages available in pkgsrc, a few hundred of them have been built on Pleiades and are available in the public directory /nasa/pkgsrc.

A new collection of software packages is released every quarter by the pkgsrc developers. In addition to new packages or updated versions, each release is largely comprised of the same packages (with identical version numbers) as previous releases.

## Software Packages Available on NAS Systems

For a list of software programs that are currently available as packages, see Available Software Modules and Packages.

You can also see which pkgsrc modules are currently available by running module avail pkgsrc. For example:

pkgsrc/2020Q4 pkgsrc/2021Q2

are available on systems running TOSS 3, and

pkgsrc/2022Q1-rome

is currently the only one available on the Aitken Rome nodes running TOSS 4.

Note: On Endeavour3/4, which still uses the SUSE Linux Enterprise Server Version 12 (SLES 12) operating system, be aware that the only pkgsrc modules available are older than 2021.

Note: Although the discussion and examples below use pkgsrc/2021Q2 and the path /nasa/pkgsrc/toss3/2021Q2, you should use pkgsrc/2022Q1-rome and the path /nasa/pkgsrc/toss4/2022Q1-rome when using the Aitken Rome nodes.

All of the source distributions for building the pkgsrc modules are stored in the/nasa/pkgsrc/distfiles directory. If you plan to build software from source, check to see whether the source distribution is already there before downloading the files from the internet.

To view a complete list of all packages and a one-line description of each package, load a pkgsrc module and type thepkg\_info command without any additional options. If you are looking for a particular package, you can check whether it is available by using the grep command plus a keyword from the output of the pkg\_info command.

TIP: Because some package names contain capital letters, add -i to the grep command to ignore case distinctions.

For example:

You can also use the -e option to test the existence of a given package. For example:

pfe% pkg\_info -e cairo

pfe% cairo-1.16.0nb4

Once you know the package name, you can use additional pkg\_info options to find more information about the package. You can specify the full package name, or you can leave out the version number. For example:

pfe% pkg\_info -B cairo-1.16.0nb4

or

pfe% pkg\_info -B cairo

Some useful options for pkg\_info include:

- -B shows build information of the package -d
- shows a long description of the package
- -L shows the files within the package
- -N shows what other packages were used to build the package
- -R shows what other packages require the package

#### **Using Packages**

The root directory of a pkgsrc release (for example, /nasa/pkgsrc/toss3/2021Q2) contains familiar directories such as bin, sbin, lib, include,

man, and info. For most packages, you can find their executables, libraries, or include files in these directories.

## **Using an Executable**

When you load a pkgsrc module, the paths to its bin and sbin directories are prepended to the PATH environment variable, as shown in the following example. Therefore, you do not need to provide full paths to these directories in order to run executables in them.

pfe% module show pkgsrc/2021Q2

/nasa/modulefiles/pkgsrc/toss3/pkgsrc/2021Q2:

/bin/logger -p local2.info -t envmodule ychang1 display pkgsrc/2021Q2 system

module-whatis A collection of software built via NetBSD's pkgsrc prepend-path INFOPATH /nasa/pkgsrc/toss3/2021Q2/info prepend-path MANPATH /nasa/pkgsrc/toss3/2021Q2/man

prepend-path PATH /nasa/pkgsrc/toss3/2021Q2/bin:/nasa/pkgsrc/toss3/2021Q2/sbin

PKGSRC\_BASE /nasa/pkgsrc/toss3/2021Q2 setenv

## **Linking a Library**

Unlike the PATH environment variable, loading a pkgsrc module does not set the LD\_LIBRARY\_PATH environment variable. The reason for this is to prevent libraries in the pkgsrc directory from overriding those with the same filenames at the system default locations or directories that may have been included in your existing LD\_LIBRARY\_PATH.

To link a static library (for example, libcairo.a) in the /nasa/pkgsrc/toss3/2021Q2/lib directory:

- -l/nasa/pkgsrc/toss3/2021Q2/include
- -L/nasa/pkgsrc/toss3/2021Q2/lib -lcairo

To link to a dynamic library (for example, libfftw.so) in the /nasa/pkgsrc/toss3/2021Q2/lib directory, follow the recommendations in the list below, in order of preference.

Note: Dynamic libraries have the suffix ".so" rather than the suffix ".a", which is used for static libraries.

• Set the LD\_RUN\_PATH environment variable as shown below prior to the link step. This will get/nasa/pkgsrc/toss3/2021Q2/lib encoded into the executable. Setting LD RUN PATH or LD LIBRARY PATH is not needed during run time.

setenv LD\_RUN\_PATH /nasa/pkgsrc/toss3/2021Q2/lib

- -l/nasa/pkgsrc/toss3/2021Q2/include
- -L/nasa/pkgsrc/toss3/2021Q2/lib -lfftw
- Add the -WI,-R linker option during the link step. This will also get/nasa/pkgsrc/toss3/2021Q2/lib encoded into the executable. Setting LD\_RUN\_PATH or LD\_LIBRARY\_PATH is not needed during run time.

Note: The linker option -WI,-R takes precedence over the LD\_RUN\_PATH setting.

- -l/nasa/pkgsrc/toss3/2021Q2/include
- -L/nasa/pkgsrc/toss3/2021Q2/lib -lfftw
- -WI,-R/nasa/pkgsrc/toss3/2021Q2/lib
- Do not set LD RUN PATH or use the -WI,-R linker option during the link step. Since/nasa/pkgsrc/toss3/2021Q2/lib is not encoded into the executable, you must set LD\_LIBRARY\_PATH during run time.

Link time:

- -l/nasa/pkgsrc/toss3/2021Q2/include
- -L/nasa/pkgsrc/toss3/2021Q2/lib -lfftw

Run time:

setenv LD\_LIBRARY\_PATH "/nasa/pkgsrc/toss3/2021Q2/lib:\$LD\_LIBRARY\_PATH"

For more information about using the setenv command, see **man setenv**.

The files of some packages are not installed in the bin, lib, and include directories. For example, the guile package is installed in the /nasa/pkgsrc/toss3/2021Q2/guile directory, which has its own bin, lib, and include subdirectories. The best way to find the exact location of a file you need from a package is to run the pkg\_info command as follows:

pfe% pkg\_info -L package\_name

Separate modules have been created for some commonly used packages to make them easier to use—you can simply load the modulefile without loading a pkgsrc module. On systems running TOSS 3, these include:

- boost/1.76
- qcc/7.5
- gcc/9.3
- gcc/10.2
- gcc/10.3
- python3/3.9.5

octave/6.2

On the Aitken Rome nodes running TOSS 4, the following modules from pkgsrc have been made available:

- boost/1.78
- gcc/6.5
- gcc/7.5
- gcc/8.4
- gcc/9.3
- gcc/10.3
- python3/3.9.12
- octave/6.4

Note: /usr/bin/python will no longer be linked to python2. To use python2, you must specify the whole path/usr/bin/python2.

Separate modules for other packages can be created when there is demand from the NAS user community.

For more information about pkgsrc, see <a href="https://www.pkgsrc.org">https://www.pkgsrc.org</a>.

#### **Using Software Modules**

See the commands described below to learn how to use modules.

Note: Software programs on NAS systems are managed either as modules or packages. For information about using software programs that are managed as packages, see <u>Using Software in the NetBSD Packages Collection</u>.

#### **Using Modules**

To find out what software modules are available on NAS systems, run the module avail command. You can also view a short description of every module by running module whatis, or find information about a specific module by running module help *modulename*.

To use the software provided in a module, you must first load the module by running the module load command. You can load several modules at the same time, as follows:

% module load module\_name\_1 module\_name\_2 ... module\_name\_N

## **Testing Modules**

New software modules and new versions of existing modules are sometimes available for testing before they are released for general use. To access the test modules, run:

module use -a /nasa/modulefiles/testing module avail module load *module name* 

If you use the test modules, please send your feedback to <a href="mailto:support@nas.nasa.gov">support@nas.nasa.gov</a>. Let us know whether the modules worked well or, if you had any problems, describe any steps you took to reproduce them.

Note: Test modules may be moved into production or deleted without notice.

#### **Additional Module Commands**

Some useful module commands include:

module list

Lists which modules are already loaded in your environment.

module purge

Removes all the modules that are loaded in your environment.

module switch old\_module\_name new\_module\_name

Enables you to switch between two modules.

module show module\_name

Shows changes that will occur in your environment if you load module\_name.

For more information, see man module.

TIP: If the module commands don't work, ensure that the following line is included in your .cshrc or .profile file:

- For csh: source /usr/local/lib/global.cshrc
- For bash: source /usr/local/lib/global.profile

## **Creating Your Own Modulefiles**

If you maintain software for your own use or to share with your group, it may be useful to create modulefiles that can be loaded, purged, and so on, just like any other modulefile.

To create your own modulefile, you can simply copy an existing modulefile to your directory (commonly named /u/your\_username/privatemodules), and edit it as appropriate.

First, find a module that you want to mimic and run module show *module\_name*. The modulefile itself will be listed at the top of the module show output. You can find most available modulefiles in the /nasa/modulefiles/toss3 directory.

Here are some common features in well-designed modulefiles:

```
#%Module
##
# All modulefiles must begin on the first line with those 8 characters
## Here, in the comments, you can describe how the package was built, or, better yet,
## put it in the ModulesHelp section below

proc ModulesHelp { } {
    puts stderr "Put the information you want to display when the user
```

```
does module help on this"
 puts stderr "modulefile. Note each continuation line begins with puts
 stderr and comments in double quotes"
# include the following line only if you want to log the loading of the
# modulefile in our system logs
# most users would leave this out
source /nasa/modulefiles/common/log_module_usage.tcl
# if there might be several versions of this software, it would be good to
#set the version number
set version 1.0-something
# setting basepath or SWDIR is for naming the root directory where your
# various bin, include, lib directories reside
# see later in the modulefile on how it is used
set basepath /u/your_userid/dir_name/dir_name
# if this software requires other modules to be loaded first,
# then use the prereq specifier, for example:
prereg comp-intel
# if your software requires other software that you build,
#then you might simply load them, as in:
module load my_other_module1 my_other_module2
# if this software conflicts with another software that the user
# may inadvertently load, then use:
conflict another_modulefile
# Finally, the actual setting of the PATHs etc. You have a choice of either
# prepend-path or append-path:
prepend-path PATH
                                      $basepath/$version/bin
prepend-path CPATH
                                      $basepath/$version/include
prepend-path FPATH
                                      $basepath/$version/include
prepend-path LD_LIBRARY_PATH
                                              $basepath/$version/lib
prepend-path LIBRARY_PATH
                                           $basepath/$version/lib
prepend-path MANPATH
                                         $basepath/$version/share/man
```

If you plan to share this software with other users in your group, make sure that they haveread permission to every file and directory, and execute permission on all directories and the executables in the software's bin directory.

In order to see your newly created modulefile in the output of the module avail command, run the module use command first, as follows:

% module use -a /u/your\_username/privatemodules

Note: The -a option puts the new modulefile at the end of module avail output. Without it, the modulefile will be listed at the top.